Determining the underlying Fermi surface of strongly correlated superconductors

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(Dated:)

The notion of a Fermi surface (FS) is one of the most ingenious concepts developed by solid state physicists during the past century. It plays a central role in our understanding of interacting electron systems. Extraordinary efforts have been undertaken, both by experiment and by theory, to reveal the FS of the high temperature superconductors (HTSC), the most prominent strongly correlated superconductors. Here, we discuss some of the prevalent methods used to determine the FS and show that they lead generally to erroneous results close to half filling and at low temperatures, due to the large superconducting gap (pseudogap) below (above) the superconducting transition temperature. Our findings provide a perspective on the interplay between strong correlations and superconductivity and highlight the importance of strong coupling theories for the characterization as well as the determination of the underlying FS in ARPES experiments.

During the last decade, Angle Resolved Photoemission Spectroscopy (ARPES) has emerged as a powerful tool [1, 2] to study the electronic structure of the HTSC [3]. This is because ARPES is a direct method to probe the FS, the locus in momentum space where the one electron excitations are gapless [4]. However, since the low temperature phase of the HTSC has a superconducting or pseudogap with d-wave symmetry, an FS can be defined only along the nodal directions or along the so-called Fermi arcs [1, 2, 5, 6, 7]. The full 'underlying FS' emerges only when the pairing interactions are turned off, either by a Gedanken experiment, or by raising the temperature. Its experimental determination presents a great challenge since ARPES is more accurate at lower temperatures. Since the FS plays a key role in our understanding of condensed matter, it is of importance to know what is exactly measured by ARPES in a superconducting or in a pseudogap state. The problem becomes even more acute in HTSC due to the presence of strong correlation effects [8, 9, 10, 11]. Hence, it is desirable to examine a reference d-wave superconducting state with aspects of strong correlation built explicitly in its construction. Motivated by these considerations, we study the FS of a strongly correlated d-wave superconductor [8, 11] and discuss our results in the context of ARPES in HTSC.

We begin by highlighting the differences between a Fermi and a Luttinger surface. The FS is determined by the poles of the one electron Green's function [4]. The Luttinger surface is defined as the locus of points in reciprocal space, where the one particle Green's

function changes sign [12]. In the Fermi liquid state of normal metals, the Luttinger surface coincides with the FS. In a Mott-Hubbard insulator the Green's function changes sign due to a characteristic $1/\omega$-divergence of the single particle self energy [13] at momenta k of the non-interacting Fermi surface. In the HTSC the gapped states destroy the FS but only mask the Luttinger surface. Hence, it seems natural to relate the Luttinger surface of the superconducting and of the pseudogap states with the concept of an 'underlying FS', and ask if such a surface can be determined by ARPES.

To answer this question, we recall that the elementary excitations in a superconductor are given by the dispersion relation,

$$E_k \;=\; \sqrt{\xi_k^2 + \Delta_k^2}, \qquad \xi_k = \epsilon_k - \mu \;, \tag{1}$$

where ϵ_k are the momentum dependent orbital energies of electrons in the absence of a superconducting order parameter Δ_k; μ is the chemical potential. The corresponding Luttinger surface is determined by the condition $\xi_k \equiv 0$, which is also the definition of the normal state FS when $\Delta_k \equiv 0$. In the following, we discuss two methods commonly used to determine the underlying FS, *viz.*, the Luttinger surface, of the HTSC by ARPES [1, 2, 14].

In the so-called 'maximal intensity method' the intensity of ARPES spectra at zero frequency is used to map out the underlying FS. It can be shown that this quantity is,

$$\sim \frac{\Gamma_k}{E_k^2 + \Gamma_k^2} \;, \tag{2}$$

where, Γ_k is determined both by the experimental resolution and the width of the quasiparticle peak. When the momentum dependence of Γ_k is small compared to that of E_k (as is usually the case), the maximal intensity is given by the set of momenta $\hbar k$ for which E_k is minimal.

To examine the accuracy of this method in determining the underlying FS, we calculate this quantity for a strongly correlated d-wave superconducting state. All calculations are done with model parameters for HTSC using the renormalized mean field theory (RMFT) [8, 11], for which the quasiparticle dispersion E_k retains the form of Eq. 1. In Fig. 1, we show our results for the spectral intensity at zero frequency as well as the locus of the Luttinger surface. The former is deduced from the inverse of E_k.

For large hole doping, $x = 0.25$, the superconducting gap is small and the Luttinger surface is close to the points in momentum space for which the zero frequency intensity is

maximal. But for smaller doping, $x = 0.05$, the gap is substantial and the Luttinger surface deviates qualitatively from the maximal intensity surface due to the momentum dependence of Δ_k (see ridges in Fig. 1). We have verified that this behaviour persists for a wide range of $|\Delta_k|$, and not just the values estimated from RMFT used in Fig. 1. Although not widely discussed in the literature, this splitting may be deduced from experimental data, *e.g.*, the intensity plots in $E-k$ space along symmetric lines $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi)$ in [15]. It follows that when the gap or the pseudogap is large, the criterion of maximal spectral intensity alone does not suffice to identify the correct FS and it is necessary to supplement the analysis of the zero frequency ARPES intensity (Eq. 2) with a dispersion relation such as Eq. 1. These considerations explain why the (outer) maximal intensity ridges seen in ARPES (at low temperatures in the underdoped regime) may yield an underlying FS whose volume is too large [16, 17].

Another method used in extracting the Luttinger surface is the 'maximal gradient method'. The method is based on the fact that the FS is given by the set of k-values for which the momentum distribution function n_k shows a jump discontinuity. When this discontinuity is smeared out, say, by thermal broadening or a small gap, the gradient of n_k, $|\nabla n_k|$, is assumed to be maximal at the locus of the underlying FS.

We calculated $|\nabla n_k|$ within RMFT and show our results in Fig. 2. We see that the maximal gradient surface is very sensitive to the presence of even small gaps. For example, the superconducting gap at $x = 0.25$ is quite small. Nonetheless, the electron-like Luttinger surface (determined by $\xi_k \equiv 0$) is not clearly revealed by the ridges in $|\nabla n_k|$. Similar deviations of $|\nabla n_k|$ from the underlying surface are also obtained from a high temperature expansion of the $t-J$ model [18] and dynamical cluster approximation in the Hubbard model [19]. We conclude that the maximal gradient method alone cannot be used to determine the underlying FS unambiguously from ARPES data.

The notion that the underlying FS of a pseudogapped or a superconducting state is identical to the Luttinger surface is only approximately correct [12, 20]. In the Fermi liquid state of normal metals, the FS satisfies the Luttinger sum rule; the volume enclosed by the FS is identical to the total number of conducting electrons. But, in a superconductor, the chemical potential is generally renormalized and is a function of the superconducting order parameter, $\mu = \mu_{SC}(\Delta)$. The number of states $n_{Lutt}(\Delta)$ enclosed by the resulting Luttinger surface, $\xi_k \equiv 0$, then deviates from the true particle number n, as the results in Fig. 3 show.

However, this effect is small (a few percent) and unlikely to be discerned experimentally. The discrepancy between $n_{Lutt}(\Delta)$ and n vanishes when particle-hole symmetry is present. Further, it changes sign when the geometry of the Luttinger surface changes from hole-like to electron-like, as seen in Fig. 3.

Finally, we focus on the influence of the strong electron-electron interactions on the geometry of the Luttinger surface close to half filling. The Cu-O planes of the HTSC are characterized by a nearest neighbor (NN) hopping parameter $t \approx 300$ meV and a next nearest neighbor (NNN) hopping parameter $t' \approx -t/4$. These parameters are the bare parameters, and determine the dispersion relation,

$$\epsilon_k \;=\; -2t\Big(\cos(k_x)+\cos(k_y)\Big) - 2t'\Big(\cos(k_x+k_y)+\cos(k_x-k_y)\Big)\;, \tag{3}$$

in the absence of any electron-electron interaction. On the other hand, true hopping processes are influenced by the Coulomb interaction $U \approx 12\,t$ leading to a renormalization of the effective hopping matrix elements,

$$t \;\;\rightarrow\;\; \tilde{t}=\tilde{t}(U), \qquad t' \;\;\rightarrow\;\; \tilde{t}=\tilde{t}'(U).$$

Close to half filling we find $\tilde{t} \propto J = 4t^2/U$ and $\tilde{t}' \rightarrow 0$, *i.e.*, the frustrating NNN hopping is renormalized to zero. This behavior is illustrated in Fig. 4. The resulting Luttinger surface renormalizes to perfect nesting. A similar behavior has been observed in recent variational studies of organic charge transfer-salt superconductors [21]. At half filling, the so-called Marshall sign rule is valid rigorously in the absence of frustration. The degree of effective frustration can then be estimated by the size of deviation from the Marshall sign rule as a function of the (frustrating) bare t'. A numerical study has found, that the Marshall sign rule remains valid even for small but finite t', *viz.*, the effective frustration renormalizes to zero [22]. This behavior is in agreement with the results presented in Fig. 4, and is unique to strong coupling theories such as RMFT.

We showed that the accurate determination of the underlying FS in underdoped HTSC is a difficult task and that analysis of the experimental data alone is often insufficient for an unambiguous determination of the FS. Commonly used methods like the zero frequency spectral intensity or the gradient of n_k can yield significant deviations from the true Luttinger surface as shown in Fig. 1 and 2. Indeed, a clear distinction between electron- and hole-like underlying FS cannot be made solely from analyses of spectral intensity maps when the gaps

are large. Such analyses have to be supplemented by a minimal modelling of the gapped states. Furthermore, the underlying FS in the pseudogapped or superconducting state fulfills Luttinger theorem only approximately, owing to the dependence of the chemical potential on the superconducting gap. We also demonstrated that the strong correlations renormalize the ratio $\tilde{t}'/\tilde{t}$ near half filling, yielding a Luttinger surface which is perfectly nested. This suggests in a very natural way that the strong coupling mean field superconducting state is unstable to antiferromagnetism at low doping. Our findings resulting from the combined effects of strong correlations and d-wave superconductivity, allow for a more precise interpretation of experiments that determine the FS of HTSC.

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[1] Damascelli, A., Hussain, Z., & Shen, Z.-X. (2003) Rev. Mod. Phys. **75**, 473.

[2] Campuzano, J. C., Norman, M. R., & Randeria, M. (2004) in *Physics of Conventional and Unconventional Superconductors*. (Springer); cond-mat/0209476.

[3] For a recent overview, see the special issue on high temperature superconductivity in Nature Physics, **2**, (March 2006).

[4] Pines, D. & Noziéres, P. (1966) *The Theory of Quantum Liquids* (Addison-Wesley).

[5] Loeser, A. G., *et al.* (1996) Science **273**, 325.

[6] Marshall, D. S., *et al.* (1996) Phys Rev Lett. **76**, 4841.

[7] Norman, M. R., *et al.* (1998) Nature **392**, 157.

[8] Edegger, B., Muthukumar, V. N., Gros, C., & Anderson, P. W. (2006) Phys. Rev. Lett. **96**, 207002.

[9] Anderson, P. W. (1987) Science **235**, 1196.

[10] Lee, P.A., Nagaosa, N., & Wen, X.-G. (2006) Rev. Mod. Phys. **78**, 17.

[11] Zhang, F. C., Gros, C., Rice, T. M., & Shiba, H. (1988) Supercond. Sci. Tech. **1**, 36.

[12] Dzyaloshinskii, I. (2003) Phys. Rev. B **68**, 085113.

[13] Gros, C., Wenzel, W., Valentí, R., Hülsenbeck, G., & Stolze, J. (1994) Europhys. Lett. **27**, 299.

[14] Mesot, J., *et al.* (2001) Phys. Rev. B **63**, 224516.

[15] Yoshida, T., *et al.* , cond-mat/0510608.

[16] In particular, this effect is seen in $Ca_{2-x}Na_xCuO_2Cl_2$ [17], which also exhibits quite a large

pseudogap [23].

[17] Shen, K. M., *et al.* (2005) Science **307**, 901.

[18] Putikka, W. O., Luchini, M. U., & Singh, R. R. P. (1998) Phys. Rev. Lett. **81**, 2966.

[19] Maier, T. A., Pruschke, T., & Jarrell, M. (2002) Phy. Rev. B **66**, 075102.

[20] Rosch, A. cond-mat/0602656.

[21] Liu, J., Schmalian, J., & Trivedi, N. (2005) Phys. Rev. Lett. **94**, 127003.

[22] Richter, J., Ivanov, N. B., & Retzlaff, K. (1994) Europhys. Lett. **25**, 545.

[23] Kohsaka, Y., *et al.* (2004) Phys. Rev. Lett. **93**, 097004.

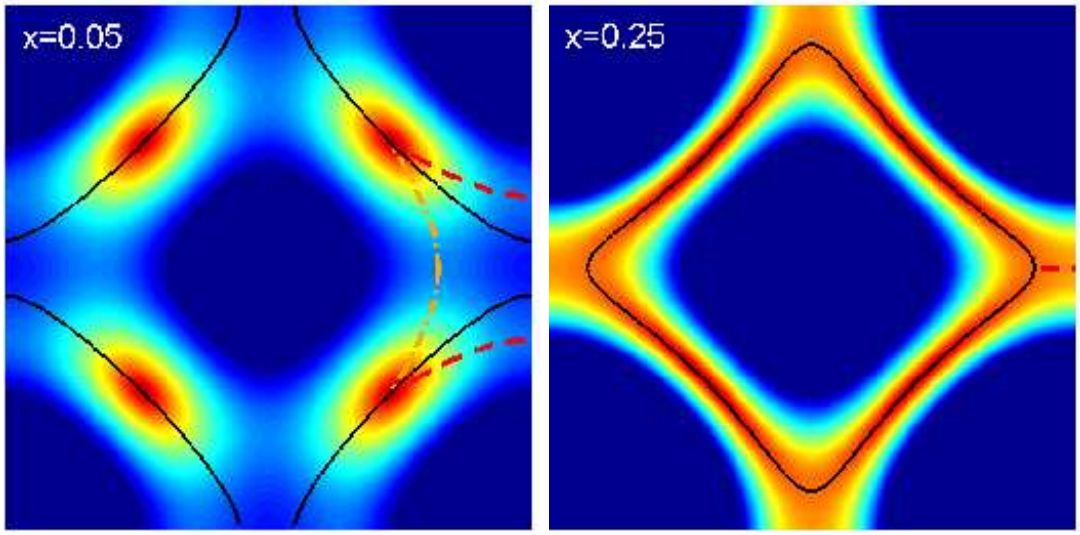

FIG. 1: The zero frequency spectral intensity (deduced from the inverse of E_k) in the first Brillouin zone for hole dopings $x = 0.05$ (left) and $x = 0.25$ (right). The color coding blue/red corresponds to the low/high zero frequency spectral intensity. The ridges of maximal intensity are indicated by the (dashed) red and (dashed-doted) orange lines respectively, the Luttinger surface by the black line.

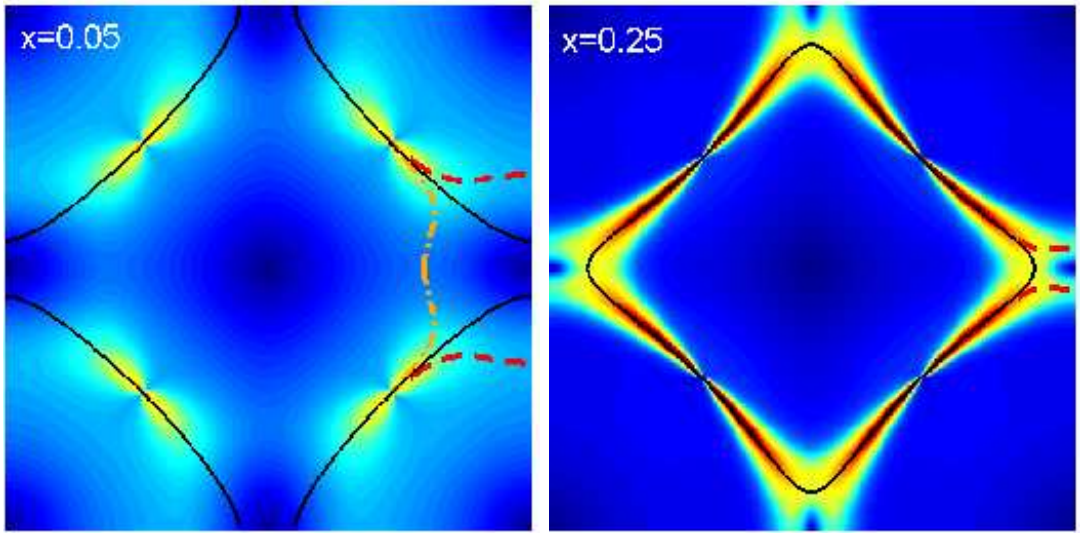

FIG. 2: The gradient of the momentum distribution function, $|n_k|$, in the first Brillouin zone, for hole dopings $x = 0.05$ (left) and $x = 0.25$ (right). The color coding is blue/red for small/large values of $|\nabla_k n_k|$. The ridges of maximal $|\nabla_k n_k|$ are indicated by the (dashed) red and (dashed-doted) orange lines respectively, the Luttinger surface by the black line.

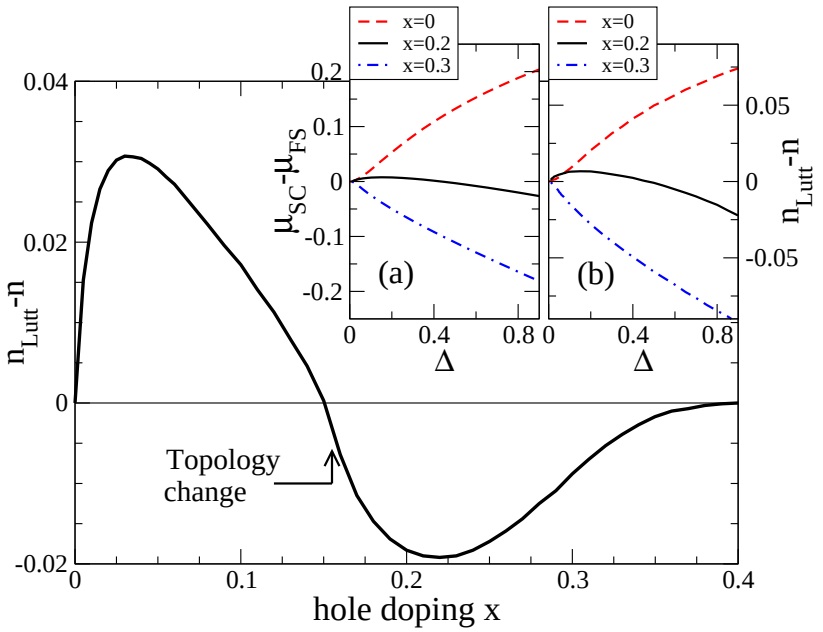

FIG. 3: The deviation, $n_{Lutt} - n$, of the actual volume of the Luttinger surface from the Luttinger sum-rule, as a function of hole-doping x. Calculations are performed by RMFT ($t' = -t/4$, $U = 12t$). The deviation is minimal when the topology of the Luttinger surface changes from hole-like to electron-like.

Inserts (a) and (b): Model calculation for the renormalization of the chemical potential, $\mu_{SC} - \mu_{FS}$, and the resulting $n_{\rm Lutt} - n$ as a function of the d-wave order Δ, for various doping x.

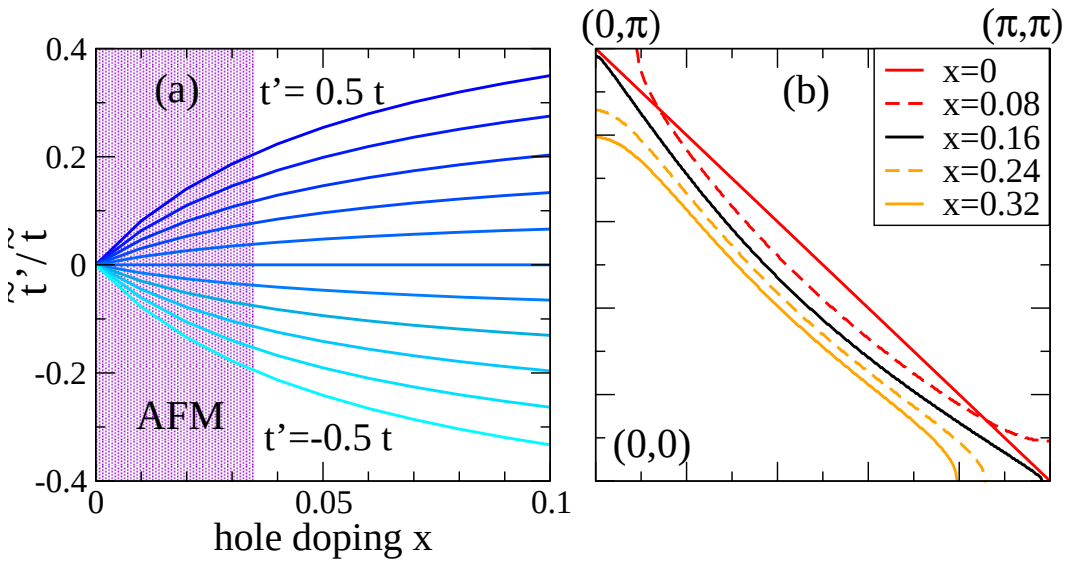

FIG. 4: (a) Renormalization of the next nearest neighbor hopping amplitude, $t' \to \tilde{t}'$, as a function of hole doping concentration x for various values of bare t'. All effective $\tilde{t}'$ are renormalized to zero at half filling by the large Coulomb repulsion. We highlight the region for which we expect the superconducting d-wave state to become unstable against antiferromagnetism (AFM) due to the nearly perfect nesting of the Luttinger surface.

(b) The geometry of the Luttinger surface for the high temperature superconductors ($t' = -t/4$). The change is non-monotonic for small doping x, when the Luttinger surface is renormalized to perfect nesting due to the strong Coulomb interaction. For $x = 0.16$, the topology of the Luttinger surface changes from hole-like to electron-like.

Calculations are performed for the Hubbard model with $U = 12t$, using RMFT.